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# Interaction of a phase front and a defect

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**Abstract.** The interaction of phase fronts and twin boundaries are observed in $NaNbO_3$ and $PbHfO_3$ single crystals. It is manifest by the stopping of a phase front by a twin boundary, as well as by their joint movement. A phase front stopped by an immovable defect of an arbitrary nature is described and expressions for the force of interaction between the defect and phase front and for the velocity of their joint movement are obtained. It is shown that (independently of the concrete defect and phase front structure) these values are determined by the difference between the free energies of the phases. The exact solution describing a phase front stopped on a narrow coherent twin boundary is obtained. It is shown that this solution exists in the whole region of the crystal phase diagram.

## 1. Introduction

Real crystals always have some defects: dislocations, dislocation walls and clusters, microcracks, inclusions and so on. Even a perfect single crystal always has at least one dislocation of growth. These defects play an important role in the phase transition (PT) process.

In crystals undergoing several structural PTs a twin structure arises during a PT at a high temperature. Twin boundaries (TBs) are defects which also play an important role if other PTs at low temperatures take place.

In this paper the interaction of a phase front (PF) and a defect is studied. The interaction is manifest by the stoppage of a PF in the vicinity of a defect as well as by tearing a defect off from locking devices and by the joint motion of a defect together with a PF. These phenomena will be called 'capture phenomena'.

It is proved theoretically that these phenomena are universal. The interaction force of a defect and a PF and the velocity of their joint motion are shown to be independent of the specific interaction mechanism (and thus of the details of the defect and PF structures) and to depend on only the difference between the free energies of the phases.

A TB is considered as a particular example of a defect which takes part in the interaction with a PF. The exact solution describing a PF stopped at a TB is obtained within the example of a PT in a crystal containing a coherent TB.

However, it is necessary to obtain experimental observations of these phenomena to confirm their existence. Direct observations of capture phenomena on TBs in $NaNbO_3$ and $PbHfO_3$ single crystals are reported here.

## 2. Observations of capture phenomena

The crystals used for the experimental investigation were plate-like and isometric $NaNbO_3$ and $PbHfO_3$ which are antiferroelectrics with sets of PTs of first order and of different

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natures:

$$Pm3m \xrightarrow{913\ K} P4/mbm \xrightarrow{848\ K} Ccmm \xrightarrow{793\ K} Pnmm \xrightarrow{755\ K} Pmnm \xrightarrow{643\ K} Pbma \underset{240\ K}{\overset{170\ K}{\rightleftarrows}} R3c$$

in $NaNbO_3$. Also the ferroelectric phases $R3c$ and $P2_1ma$ can be induced in $NaNbO_3$ by an electric field [1, 2]. The transitions

$$Pm3m \xrightarrow{473\ K} P222_1 \xrightarrow{440\ K} Pba2$$

take place in $PbHfO_3$ [3]. The experimental details and the descriptions of different phases, PFs and TBs observed in these crystals have been reported elsewhere [2–4].

In $NaNbO_3$ crystals a PT can both be followed by twin-structure reconstruction and take place without reconstruction of the twin structure. In the first case the capture of the TB by the PF was observed, the TB being moved in the crystal in the vicinity of the PF in the direction of its motion.

Capture of the PF by the TB was also observed. In this case the PF was coming towards the TB and was stopped in its vicinity (at an invariable electric field value in the case of the induced PT and at a constant temperature value for the temperature PT). If the electric field was increased again (or the temperature was changed), the PF was observed to be torn off the TB and to continue its motion in the crystal.

The capture phenomena of the TBs {110} and {1$k$1} were observed under the transition $Pbma \rightarrow R3c$ and of the TBs {100}, {110} and {1$k$1} under the transitions $Pbma \rightarrow P2_1ma$ and $Pbma \rightarrow Pmnm$. The fragments of the PTs $Pbma \rightarrow P2_1ma$ and $Pbma \rightarrow Pmnm$ with the capture phenomena in $NaNbO_3$ are displayed in figures 1 and 2.

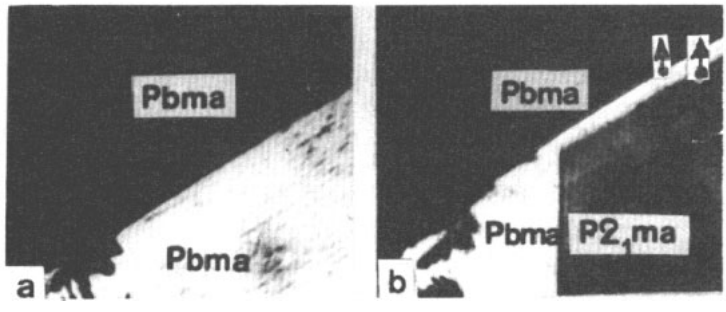


**Figure 1.** Micrographs of a $NaNbO_3$ crystal undergoing the PT $Pbma \rightarrow P2_1ma$, induced by an external electric field. (*a*) The TB {1$k$1} in the phase Pbma. (*b*) The joint movement of the TB and the PF (the direction of movement is indicated by arrows).

In the plate-like $PbHfO_3$ crystals the first-order PT between the paraelectric cubic phase $Pm3m$ and the orthorhombic antiferroelectric phase $P222_1$ was investigated.

Several types of 90° and 60° flat and zigzag TBs were observed in the $P222_1$ phase of $PbHfO_3$ crystals [4]; however, only flat 60° TBs which are situated along the {110} plane of the pseudocubic cell took part in the interaction with the PF.

The capture of a TB was observed only if the region of the low-symmetry phase was twinned and had one or several 60° TBs which made an acute angle with a PF.

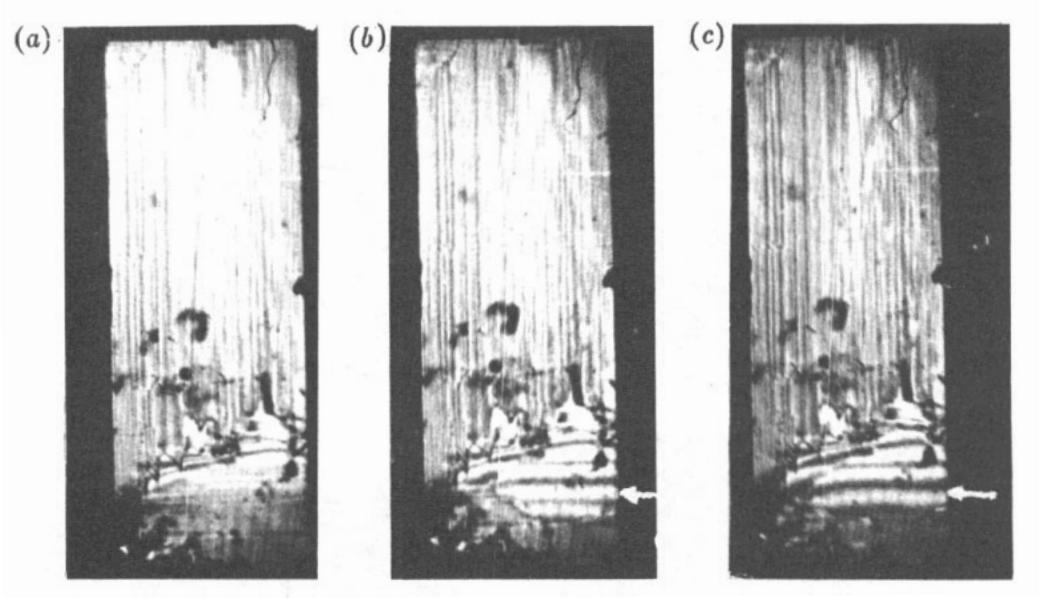


**Figure 2.** Photographs of the fragments of the PT $Pmnm \rightarrow Pbma$ in a $NaNbO_3$ crystal. (*a*) The twinned phase $Pmnm$ and the PF of the $Pbma$ phase (at the bottom of the picture). (*b*), (*c*) Movement of the TB under the PF action. The TB is tilted with respect to the picture plane (to the crystal edge) and can be seen as the set of parallel diffuse interference bands (indicated by arrows). The TB displacement can be measured from the defects which can be seen on the photographs.

The set of micrographs showing the PT $Pm3m \rightarrow P222_1$ in $PbHfO_3$, which is followed by the capture of a 60° TB {110} by the PF, situated along the plane {520} of the pseudocubic cell, is displayed in figure 3. This PF is the zero net strain plane [3].

The 60° TB (indicated by an arrow in figure 3(*a*)) divides the orthorhombic phase region into two parts (I and II) with different constrasts and intersects the PF. With decreasing temperature the orthorhombic phase region increases, the intersection of the TB and the PF being moved to the left edge of the crystal (figures 3(*b*)–(*d*)). After the intersection had arrived at the crystal edge, the TB tore itself off the PF and their joint motion was stopped. Note that small 60° wedges arise in the PT process in the vicinity of the intersection of the TB and the PF (figure 3(*c*)). This indicates the existence of mechanical stress in this region. The wedges disappear after the TB has been torn off the PF.

The 90° TB of the orthorhombic phase does not influence capture phenomena.

The observations reported make it possible to see that the capture phenomena exist in different crystals for PTs of different natures. Thus it is reasonable to suppose that interaction between a PF and a TB has universal features. The universal features of this interaction are discussed here in the framework of the Landau theory of PTs.

## 3. Theoretical description of capture phenomena

Consider a crystal containing defects which experiences a PT of the first order on decreasing the temperature. Defects can either favour or resist the PT. When the crystals is supercooled, the PF jumps off defects of the first kind and moves inside the crystal until it reaches defects

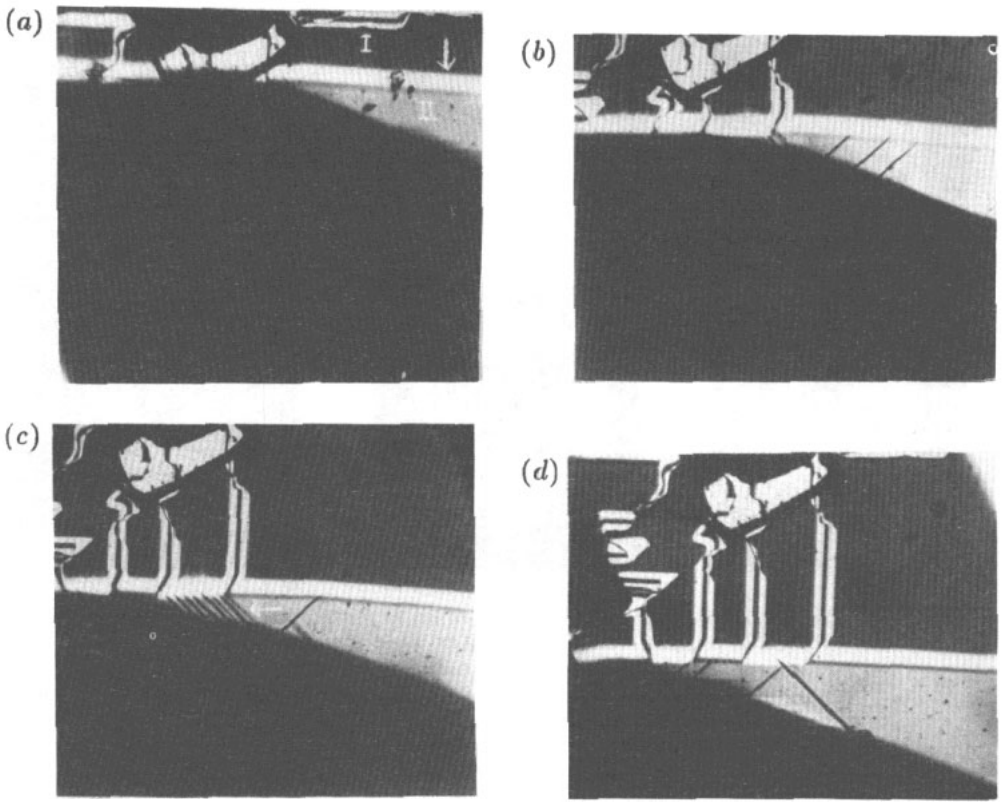


Figure 3. The fragments of the PT $Pm3m \rightarrow P222_1$ in a $PbHfO_3$ crystal: I, the phase $P222_1$ region with symmetric extinction; II, region with parallel extinction. The arrows indicate the 50° twin boundary (which is parallel to the {110} plane of a pseudocubic cell) in (*a*) and small 50° wedges in (*c*).

of another kind, which are able to take part in the capture phenomena. These are defects increasing the 'local temperature' and defects of 'local field' type. The defects which often generate a low-temperature phase are crystal edges but they can also be generated by TBs [5–7], dislocations [9], cracks [10] and so on. In this paper the PF which has jumped off the crystal edge is considered.

Consider the interaction of a defect with a flat PF in the crystal which is supposed to have the form of a right-angled parallelepiped, the PF being perpendicular to the $Ox$ direction.

In the most general case the PT is described by the $n$-component order parameter (OP) $\eta_i$ $(i = 1, 2, \ldots, n)$.

The free energy has the form

$$F = \int \left( \tfrac{1}{2} g \sum_{i=1}^{n} (\nabla \eta_i)^2 + \varphi(\eta_i) \right) \mathrm{d}V + F_{\mathrm{int}}(\xi) \tag{1}$$

where $g > 0$ is a constant and

$$\varphi(\eta_i) \equiv \varphi(\eta_1, \eta_2, \ldots, \eta_n)$$

is the free energy density of the homogeneous crystal; $\varphi(0) = 0$. $V$ is the crystal volume and $F_{\mathrm{int}}(\xi)$ is the part of the free energy describing the interaction with the defect which

depends on the defect coordinate $\xi$. The method for introducing the defect coordinate depends on the nature of the defect. Several examples will be considered later. In the most general case the interaction term can be written in the form

$$F_{\text{int}} = \int_V \sum_{i=1}^{n} \eta_i^k U_i(x-\xi, y, z)\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z. \tag{2}$$

Note that equation (2) is the most general form of the interaction of the OP and the defect of an arbitrary nature. If the defect is of the 'local temperature' type, in this case $k = 2$ and, if the defect is of the 'local field' type conjugated to all or to some OP components, in this case $k = 1$. In the general case this 'local field' acts differently on the different OP components; thus in a general case, $U_1 \neq U_2 \neq \ldots \neq U_n$. Here the functions $U_i(x-\xi, y, z)$ describe the interaction of the OP and the defect. They appear as the result of the OP interaction with some other degrees of freedom which are not equal to zero in the vicinity of the defect (e.g. the strain field, other OPs, and distribution of point defects).

Consider several examples of possible interaction of a defect and an OP field.

The case of a PT in a crystal containing a wide coherent TB (domain wall) was considered in [8]. It was shown that the interaction term had the form

$$F_{\text{int}} \sim \int \eta^2 \cosh^{-2}[(x-\xi)/l_{\text{TB}}]S\,\mathrm{d}x$$

where $l_{\text{TB}}$ is the TB width and $S$ is the TB area.

The narrow coherent TB model was considered to describe the nucleation on a TB during a PT into a superconducting phase [5] and during structural PTs [6, 7]. In both cases the interaction term is

$$F_{\text{int}} = A \int \eta^2 \delta(x) S\,\mathrm{d}x$$

where $A$ is the TB power and $\delta(x)$ is the $\delta$-function. This model can be obtained from the first model in the case $l_{\text{TB}} \ll r_c$, where $r_c$ is the OP correlation radius [5, 8]. Note that in both cases [5–8] at least two different OPs were considered in the theory directly or the second OP was implied. The first OP is $\eta$. It describes the low-temperature PT. The other OP describes the high-temperature PT. If TBs appear in the crystal under the high-temperature PT, then the distribution of this OP is inhomogeneous [8]. The inhomogeneities in this OP distribution describing the TB give rise to the inhomogeneous term in the free energy [8].

Consider the case of an elastic defect (in other words the case of a defect which gives rise to the inhomogeneous elastic field $u_{ij}(r)$, where $u_{ij}(r)$ is the strain tensor). In the case of a PT with multiplication of the elementary cell (except improper ferroelastics) there is only one striction term and the interaction part of the free energy should be written

$$F_{\text{int}} = A \int \sum_{i=1}^{n} \eta_i^2 u_{ll}(x-\xi, y, z)\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z$$

where $A$ is the striction constant.

In the case of improper ferroelastics (e.g. in the case of ferroelectrics) there can be several invariants of this kind in the free energy which are linear in $u_{ij}(r)$ and of the second order in $\eta$ [11]. Thus the case $k = 2$ occurs.

Finally in the case of ferroelastics the interaction term is linear in both the OP and the strain tensor (the case $k = 1$).

The particular strain field distribution has different forms for defects of different kinds.

In the case of the edge dislocation stretched along Oz with the coordinates $x = \xi$, $y = 0$, the trace of the strain tensor has the form

$$u_{ll} = [b(1-2\nu)/2\pi(1-\nu)][y/((x-\xi)^2+y^2)]$$

where $b$ is the Burgers vector and $\nu$ is Poisson's ratio [12, 13].

In the case of a flat crack lying in the $x$–$y$ plane with its tip at the point $x = \xi$, $y = 0$ the trace of the strain tensor has the form

$$u_{ll} = B\cos(\varphi/2)/r^{1/2} = B\{[(x-\xi)^2+y^2]^{-1/2} + [(x-\xi)^2+y^2]^{-1}\}^{1/2}$$

where

$$B = 2K_I(1-2\nu)(1+\nu)/(2\pi)^{1/2}E.$$

Here $K_I$ is the stress intensity factor, $E$ is Young's modulus, and $r$ and $\varphi$ are the cylindrical coordinates measured from the crack tip [10].

The incoherent TB is often considered as a wall of equidistant dislocations [13]. In the case of a dislocation wall which is parallel to the $y$–$z$ plane with the coordinate $x = \xi$ (the dislocations being parallel to the Oz axes) the strain tensor trace takes the form

$$u_{ll} \approx \exp(-2\pi|x-\xi|/h)\sin(2\pi y/h)$$

where $h$ is the distance between the dislocations [13].

These expressions should be substituted into $F_{int}$ in order to calculate the interaction energy for a defect of particular type. In the cases considered, the functions $U_i$ depend on only two coordinates (in the geometry considered, they are $x$ and $y$). However, a dependence on three coordinates can also occur in the case of a more complicated defect.

These examples show some particular realizations of inhomogeneities giving rise to the interaction term $F_{int}$. However, in this paper the general properties of capture phenomena are studied. They are independent of the specific structure of the defect.

The condition of the potential (1) minimum results in the equation of state

$$g(\partial^2\eta_i/\partial x^2 + \partial^2\eta_i/\partial y^2 + \partial^2\eta_i/\partial z^2) = \partial\varphi/\partial\eta_i + k\eta_i^{k-1}U_i(x-\xi, y, z) \quad (3)$$

and the boundary conditions on the crystal surface

$$(\boldsymbol{n}\cdot\nabla)\eta_i = 0 \quad (4)$$

where $\boldsymbol{n}$ is the normal unit vector and $\nabla$ is the gradient operator.

It is not difficult to see that the force $f = -\partial F/\partial\xi$ acts in a general case from the OP field to the defect:

$$f = -\sum_{i=1}^{n}\int \frac{\partial\eta_i^k}{\partial x}U_i(x-\xi, y, z)\,dx\,dy\,dz. \quad (5)$$

The solution describing the PF stopped at the defect has the asymptotics

$$\eta_i(-\infty, y, z) = \eta_i^{(0)} \qquad \eta_i(+\infty, y, z) = 0 \quad (6)$$

which are the additional boundary conditions. Here $\eta_i^{(0)}$ are the solutions of the equations of state $\partial\varphi/\partial\eta_i = 0$ in the corresponding homogeneous phase $\eta =$ constant $\neq 0$.

Nucleation on 'local temperature' type of defects can take place at a higher temperature than the PT temperature if the contribution of the last term in (1) is negative. As a result, capture phenomena can take place in the opposite case for $f > 0$. Suppose that the PF is flat (the PF bending in the defect field can be neglected for PTs of first order) and that the OP distribution has the form of a step $\eta = \eta(x - \xi_0)$; $\partial\eta/\partial x \sim \eta^{(0)}\delta(x - \xi_0)/l_{PF}$ (where $\xi_0$ is the PF coordinate, and $l_{PF}$ is the PF width); then one can obtain an estimation for the condition for capture phenomena to occur:

$$\sum_{i=1}^{n}(\eta_i^{(0)})^k \int U_i(\xi_0 - \xi, y, z)\,dy\,dz > 0.$$

Obviously, in the case of a perfect crystal (one obtains this case by taking $U_i = 0$) the solution of equation (3) with the boundary conditions (4) and (6) exists only at the first-order PT point, because the asymptotics $\eta_i(-\infty, y) = \eta_i^{(0)}$ and $\eta_i(+\infty, y) = 0$ correspond to different values of the first integral of equation (3). The condition of equality of these first integrals gives the equation of a line in the phase diagram which is the line of the first-order PT. Thus a solution describing a motionless PF does not exist for a perfect crystal away from first-order PT line. On the other hand in the two-phase region of the phase diagram for the perfect crystal out of the first-order PT line a solution describing the moving phase front exists.

However, in the case of a crystal containing a defect the solution with the asymptotics (4) and (6) can exist in some region in the phase diagram.

Equations (3) should be multiplied by $\partial\eta_i/\partial x$, integrated over $x$ and $y$ and summed over $i$. Using the relations

$$(\partial\eta_i/\partial x)(\partial^2\eta_i/\partial z^2) = (\partial/\partial z)[(\partial\eta_i/\partial z)(\partial\eta_i/\partial x)] - \tfrac{1}{2}(\partial/\partial x)(\partial\eta_i/\partial z)^2$$

$$(\partial\eta_i/\partial x)(\partial^2\eta_i/\partial y^2) = (\partial/\partial y)[(\partial\eta_i/\partial y)(\partial\eta_i/\partial x)] - \tfrac{1}{2}(\partial/\partial x)(\partial\eta_i/\partial y)^2$$

and

$$(\partial\eta_i/\partial x)(\partial^2\eta_i/\partial x^2) = \tfrac{1}{2}(\partial/\partial x)(\partial\eta_i/\partial x)^2$$

one can see that the left-hand part of the equation becomes zero after integration because of the boundary conditions (4). Taking into account that

$$\int_{\infty}^{\infty} dx \int_{-L_y/2}^{L_y/2} dy \int_{-L_z/2}^{L_z/2} dz \left( \sum_{i=1}^{n} \frac{\partial\varphi}{\partial\eta_i}\frac{\partial\eta_i}{\partial x} \right) = [\varphi(\eta_i(\infty) - \varphi(\eta_i(-\infty))]L_zL_y = -\varphi(\eta_i^{(0)})S$$

(where $L_y$ and $L_z$ are the crystal sizes in the Oy and Oz directions, and $S = L_zL_y$ is the crystal area of the cross section which is perpendicular to the Ox direction) using (5) one can finally obtain

$$f = -\varphi(\eta_i^{(0)})S. \tag{7}$$

(It should be noted that this result is obtained for arbitrary $U_i$ functions. Thus it can be applied to defects of all types interacting with the OP, for which the capture condition is fulfilled.)

The fulfilment of this condition is necessary but is not sufficient, however, for the existence of a solution of equations (3), (4) and (6). Thus it is necessary to show that such a solution can be obtained exactly at least in the framework of a simple model.

## 4. The exact solution of a phase front stopped at a narrow coherent twin boundary

The exact solution is obtained here in the particular case of a simple model of a coherent narrow TB. As is discussed above in the case of a narrow TB which is perpendicular to the $Ox$ direction, the functions $U_i$ can be taken in a form

$$U_i(x-\xi, y, z) = A\delta(x-\xi)$$

being the same for all $i = 1, 2, \ldots, n$.

Consider the case of the first-order PT describing by a one-component OP $\eta$. In this case, $n = 1$ and

$$\varphi(\eta) = \tfrac{1}{2}\alpha\eta^2 + \tfrac{1}{4}\beta\eta^4 + \tfrac{1}{6}\gamma\eta^6 \tag{8}$$

where $\alpha$, $\beta$ and $\gamma$ are the phenomenological constants, with $\gamma > 0$, $\beta < 0$, $\alpha = a(T - T_c)$ $(a > 0)$.

The equilibrium equation which follows from the minimum condition of the free energy has the form

$$g(\partial^2\eta/\partial x^2) = \alpha\eta + \beta\eta^3 + \gamma\eta^5 + kA\eta^{k-1}\delta(x-\xi). \tag{9}$$

The solution describing the PF stopped on the motionless TB must have the asymptotics $\eta(-\infty) = \eta_0$, $\eta(+\infty) = 0$ and $\eta'(\pm\infty) = 0$ and must be continuous, but the derivative has a jump at the point $x = \xi$ because of the singular term in equation (9).

The exact solution has the form

$$\eta^2 = \begin{cases} 12\alpha/\{(9\beta^2 - 48\alpha\gamma)^{1/2}\cosh[2(\alpha/g)^{1/2}(x-\xi) + q] + 3|\beta|\} & x \geqslant \xi \\ [\eta_0^2 b^2 \sinh^2(t+p)]/[\eta_0^2 + b^2\cosh^2(t+p)] & x < \xi. \end{cases} \tag{10}$$

where

$$\eta_0^2 = [-\beta + (\beta^2 - 4\alpha\gamma)^{1/2}]/2\gamma$$
$$b^2 = [\beta + 2(\beta^2 - 4\alpha\gamma)^{1/2}]/2\gamma$$
$$t = \eta_0[4(\beta^2 - 4\alpha\gamma)/2g^2]^{1/4}(x-\xi).$$

The constants $p$ and $q$ should be determined from the conditions on the TB (see appendix). These conditions give the system of the transcendental algebraic equations for $p$ and $q$. It is important to show that they have a solution in some region of the phase diagram. If the existence of this solution is proved and the region of its existence is found, then it is the phase diagram region where a capture phenomenon can take place. The $p$- and $q$-values in this region can be found approximately.

The solution (10) can obviously exist only in the two-phase region of a phase diagram: between the lines $\alpha = \beta^2/4\gamma$ (figure 4, line 1) and the line $\alpha = 0$. However, the solutions for $p$ and $q$ (appendix) exist in a smaller part of the phase diagram, which is displayed in figure 4 on the background of the phase diagram of the potential (8). It is situated between lines 3 and 4 (figure 4), given by the expressions

$$2\sqrt{6}A\gamma(g|\beta|^3)^{-1/2} = 2m\sqrt{m} + K \tag{11}$$

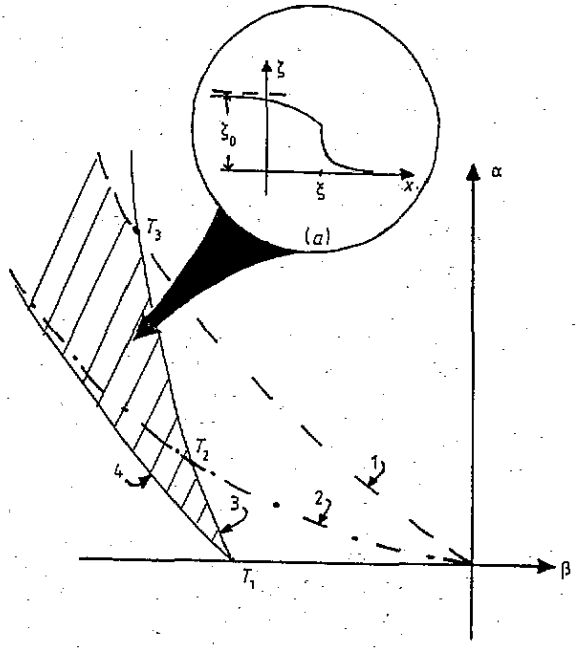


**Figure 4.** The region of existence of the solution (10) (shaded) on the background of the phase diagram of the potential (8): line 1, the line $\alpha = \beta^2/4\gamma$, the two-phase region boundary; line 2, the line $\alpha = 3\beta^2/16\gamma$, the first-order PT line; line 3, line given by (11); line 4, line given by (12), the boundaries of the region of existence of the solution (10). (*a*) The solution (10), describing the phase front, stopped at the TB.

and

$$2\sqrt{6}A\gamma(g|\beta|^3)^{-1/2} = 2m\sqrt{m} - K \tag{12}$$

respectively. Here $K = (2m^3 - 3m^2 + 1)^{1/2}$ and $m = (1 - 4\alpha\gamma/\beta^2)^{1/2}$.

Line 3 (figure 4) intersects the line $\alpha = 0$, the line $\alpha = 3\beta^2/16\gamma$ (the line of the first-order PT; figure 4, line 2) and the line $\alpha = \beta^2/4\gamma$ at the points $T_1$, $T_2$ and $T_3$, respectively (figure 4). The coordinates of these points are

$$|\beta_1^3| = 6A^2\gamma^2/g \qquad |\beta_2^3| = 12A^2\gamma^2/g \qquad |\beta_3^3| = 24A^2\gamma^2/g. \tag{13}$$

Line 4 (figure 4) intersects line $\alpha = 0$ at the point $T_1$ and for $\beta \to -\infty$ coincides with line 2. Thus a region in the phase diagram exists in which the solution (10) of equation (9) occurs.

In the cases of other, more complicated models of TBs, one can hardly hope to obtain the analytic solution of equation of state describing the stopped PF, but the exact result obtained in the framework of this sample model makes it possible to expect that solutions of the same type take place in a general case.

## 5. Joint motion of the twin boundary and phase front

If the pressure $\sigma$ of the force $f$ ($\sigma = f/S$) is more than $\sigma_*$ (the maximum value of the pressure due to the interaction of a TB with locking devices or due to the Peierls force), the TB can be moved by the PF.

The dissipative function for the case of an $n$-component OP has the form

$$\Psi = \frac{\kappa}{2}\sum_{i=1}^{n}\int\left(\frac{\partial\eta_i}{\partial t}\right)^2 \mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z. \tag{14}$$

The equation of motion of the OP resulting from (1), (2) and (14) is

$$\kappa(\partial\eta_i/\partial t) = g(\partial^2\eta_i/\partial x^2 + \partial^2\eta_i/\partial y^2 + \partial^2\eta_i/\partial z^2) - \partial\varphi/\partial\eta_i - k\eta_i^{k-1}U_i(x-\xi, y, z) \tag{15}$$

where $t$ is the time and $\xi = \xi(t)$. The solution should be tried in the form $\eta = \eta(x-\xi(t), y, z)$. Substituting this expression into (15), multiplying by $\partial\eta_i/\partial x$, summing over $i$ and integrating over $x$, $y$ and $z$ as was done before, one can obtain the equation for $\xi(t)$:

$$\kappa J(\partial\xi/\partial t) = -\varphi(\eta_i^{(0)}) - \sigma_* \tag{16}$$

for $|\varphi(\eta_i^{(0)})| - \sigma_* > 0$. In the case $T < T_0$, one can obtain $\varphi(\eta_0) < 0$ and thus $f > 0$. ($T_0$ is the temperature of the first-order PT. In the case of the PT described by the potential (8) the PT takes place on the line $\alpha = 3\beta^2/16\gamma$ of the phase diagram; thus $T_0 = T_c + 3\beta^2/16\gamma a$.) Here

$$J = \sum_{i=1}^{n}\int_{-\infty}^{\infty}\left(\frac{\partial\eta_i}{\partial x}\right)^2 \mathrm{d}x \tag{17}$$

and the value of the integral $J$ can be estimated as $J \sim \sum(\eta_i^{(0)})^2/l_{\mathrm{PF}}$.

Note that the results (7) and (16) are universal; they do not depend on the concrete mechanism of the interaction of TB and the OP and on the structure of the free energy (1) (the polynomial (8) power, the number of components for the OP and so on). However, the form of the exact solution (10) of the equation of state (9) and the region of existence of this solution are determined by the potential structure (1) and (8).

The maximum value of the pressure $\sigma$ can be obtained on the edge of the two-phase region of the phase diagram. In the case of the transition described by the potential (1) and (8) it occurs at $\alpha = 0$; hence it follows that $\sigma_{\max} = |\beta|^3/12\gamma^2$.

At $\alpha < 0$ the solution (10) does not exist. Thus for supercooling $\alpha < 0$, the PF is torn off the TB and the whole crystal becomes a low-symmetry phase.

The condition $|\varphi(\eta_i^{(0)})| \equiv |\varphi(T_1)| = \sigma_*$ gives the temperature $T_1$ at which the PF tears the TB off the locking devices. At the small value $T - T_1 < 0$ the velocity of the joint movement of the PF and the TB has the form

$$\partial\xi/\partial t = s(T_1 - T)/\kappa J \tag{18}$$

where the transition entropy density $s = -\partial\varphi/\partial T$. In the case described by the potential (8), $s = a\eta_0^2/2$.

The values of the constants of the potentials which describe the transitions in $NaNbO_3$ and $PbHfO_3$ are unknown. However, one can estimate the values of $\sigma$ and $\partial\xi/\partial t$ using the experimental data for some ferroelectrics [14]. One can obtain $\sigma_{\max} \sim 10^3$–$10^4$ Pa [14]. Using the values $a \sim 10^5$ J m s C$^{-2}$ K$^{-1}$ [14], $l \sim 10^{-10}$ m, $\kappa \sim 10^{-5}$–$10^{-6}$ J m s C$^{-2}$ (which corresponds to a relaxation time of about $10^{-10}$–$10^{-11}$ s), one can obtain $s/\kappa J \sim$ 1–10 m s$^{-1}$ K$^{-1}$.

## Appendix. The solution of equation (9)

After the transformations

$$x - \xi = z(g\gamma)^{1/2}/|\beta| \qquad \alpha = u\beta^2/\gamma \qquad \eta = \theta(z)(|\beta|/\gamma)^{1/2}$$

equation (9) for the case $k = 1$ is reduced to the form

$$\partial^2\theta/\partial z^2 = u\theta - \theta^3 + \theta^5 + D\delta(z) \tag{A1}$$

where $D = A\gamma(g|\beta|^3)^{-1/2}$. The solution of equation (A1) must be continuous with a jump of $\theta'(0)$. Integrating equation (A1) over $z$ from $-\epsilon$ to $\epsilon$ and taking the limit $\epsilon \to 0$, one can obtain the conditions which must be fulfilled at the point $z = 0$:

$$\theta'(+0) - \theta'(-0) = D. \tag{A2}$$

The continuity condition has the form

$$\theta(+0) = \theta(-0). \tag{A3}$$

The expression for the force $f$, obtained with the help of (5), is

$$(AS/2\gamma)(|\beta|^3/g)^{1/2}[\theta'(+0 + \theta'(-0)] = f. \tag{A4}$$

Equations (A1)–(A4) together with equation (7) for the force are the complete system which makes it possible to obtain the solution with the asymptotics (4) and (6). Equation (A1) is conservative everywhere except for at the point $z = 0$. Thus the first integrals exist; one of them is equal to zero and corresponds to the first expression in equation (10), and the second, which is equal to $-\tilde{\varphi}(\theta_0)$, corresponds to the second expression in equation (10). Here $\varphi(\eta) = |\beta^3|\tilde{\varphi}(\theta)/\gamma^2$. These two expressions must satisfy equations (A2)–(A4) and (7) at the point $z = 0$. They can be reduced to

$$\begin{aligned} \theta'(+0) &= \tilde{\varphi}(\theta_0)/D + \tfrac{1}{2}D \\ \theta'(-0) &= \tilde{\varphi}(\theta_0)/D - \tfrac{1}{2}D \end{aligned} \tag{A5}$$

where $\theta_0^2 = \frac{1}{2}[1 + (1 - 4u)^{1/2}]$. Equation (A5) is the system of transcendental equations which makes it possible to obtain the values of the constants $p$ and $q$ for the solution (10). The left-hand parts of both equations (A5) are limited; thus the condition of existence of the solution of (A5) for $p$ and $q$ is

$$|[\theta'(\pm 0)]|_{\max} \geqslant \tilde{\varphi}(\theta_0)/D \pm \tfrac{1}{2}D. \tag{A6}$$

The inequalities (A6) give the region of existence of the solution (10) in the phase diagram. The boundaries of this region are given by (11) and (12). In this region the solution exists and the values of $p$ and $q$ can be obtained approximately.

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